Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 05:00 pm BST

PDB ID	:	1D01
Title	:	STRUCTURE OF TNF RECEPTOR ASSOCIATED FACTOR 2 IN COMPLEX WITH A HUMAN CD30 PEPTIDE
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Deposited on	:	1999-09-07
Resolution	:	2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

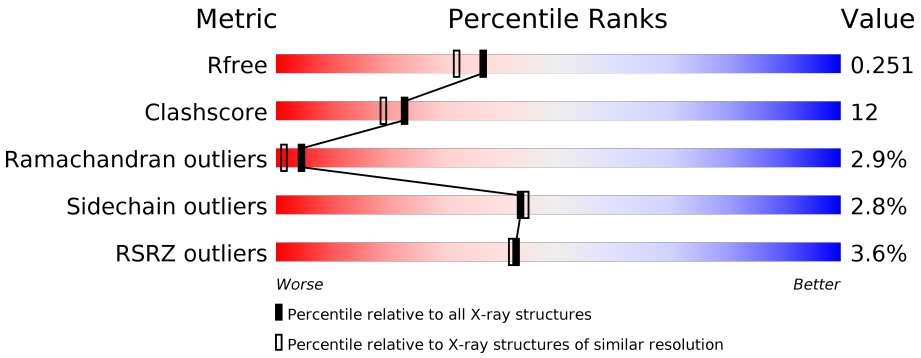
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	168	3% 82% 15% ·
1	B	168	3% 79% 18% ·
1	C	168	2% 80% 17% ·
1	D	168	4% 77% 21% ·
1	E	168	4% 80% 16% ·
1	F	168	6% 77% 20% ·

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Mol	Chain	Length	Quality of chain
2	G	9	89% 11%
2	H	9	78% 22%
2	I	9	78% 22%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8705 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called TUMOR NECROSIS FACTOR RECEPTOR ASSOCIATED FACTOR 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	168	Total	C	N	O	S	0	0	0
			1282	825	217	231	9			
1	B	168	Total	C	N	O	S	0	0	0
			1282	825	217	231	9			
1	C	168	Total	C	N	O	S	0	0	0
			1282	825	217	231	9			
1	D	168	Total	C	N	O	S	0	0	0
			1282	825	217	231	9			
1	E	168	Total	C	N	O	S	0	0	0
			1282	825	217	231	9			
1	F	168	Total	C	N	O	S	0	0	0
			1282	825	217	231	9			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	365	ARG	LEU	CONFLICT	UNP Q12933
B	365	ARG	LEU	CONFLICT	UNP Q12933
C	365	ARG	LEU	CONFLICT	UNP Q12933
D	365	ARG	LEU	CONFLICT	UNP Q12933
E	365	ARG	LEU	CONFLICT	UNP Q12933
F	365	ARG	LEU	CONFLICT	UNP Q12933

- Molecule 2 is a protein called CD30 PEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	9	Total	C	N	O	S	0	0	0
			62	38	8	15	1			
2	H	9	Total	C	N	O	S	0	0	0
			62	38	8	15	1			
2	I	9	Total	C	N	O	S	0	0	0
			62	38	8	15	1			

- Molecule 3 is water.

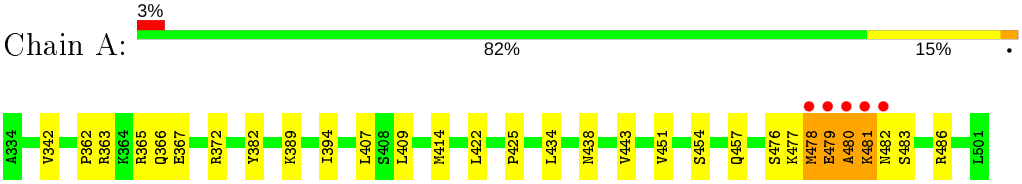
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	145	Total O 145 145	0	0
3	B	143	Total O 143 143	0	0
3	C	136	Total O 136 136	0	0
3	D	116	Total O 116 116	0	0
3	E	128	Total O 128 128	0	0
3	F	125	Total O 125 125	0	0
3	G	14	Total O 14 14	0	0
3	H	9	Total O 9 9	0	0
3	I	11	Total O 11 11	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

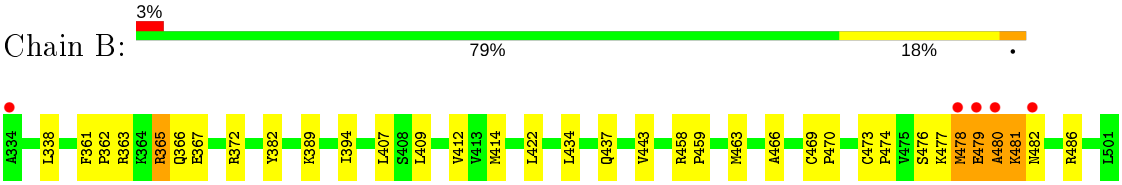
- Molecule 1: TUMOR NECROSIS FACTOR RECEPTOR ASSOCIATED FACTOR 2

Chain A:



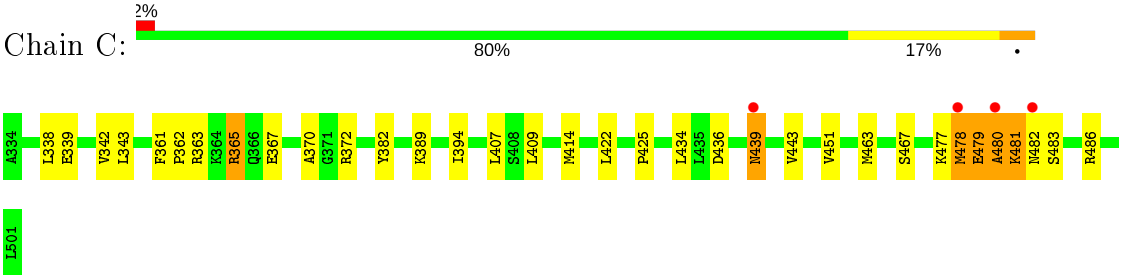
- Molecule 1: TUMOR NECROSIS FACTOR RECEPTOR ASSOCIATED FACTOR 2

Chain B:



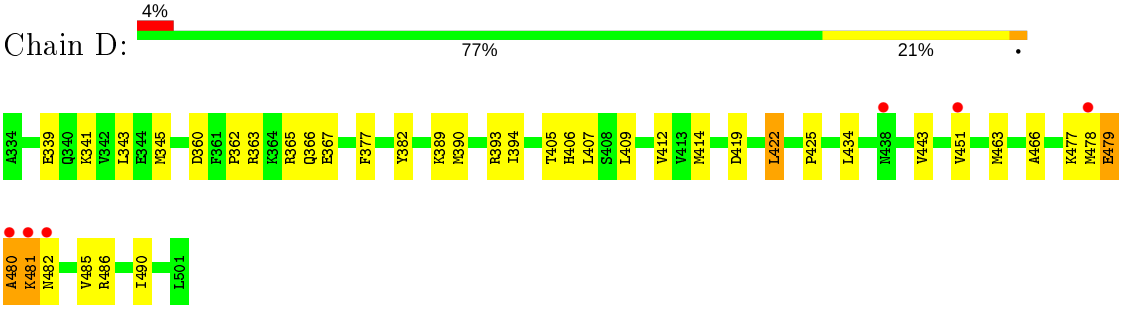
- Molecule 1: TUMOR NECROSIS FACTOR RECEPTOR ASSOCIATED FACTOR 2

Chain C:



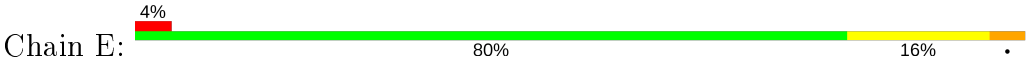
- Molecule 1: TUMOR NECROSIS FACTOR RECEPTOR ASSOCIATED FACTOR 2

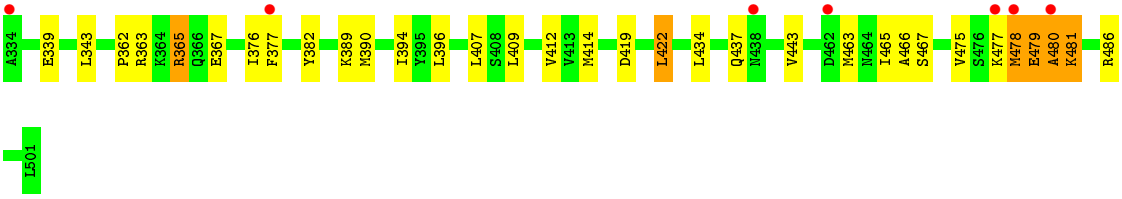
Chain D:



- Molecule 1: TUMOR NECROSIS FACTOR RECEPTOR ASSOCIATED FACTOR 2

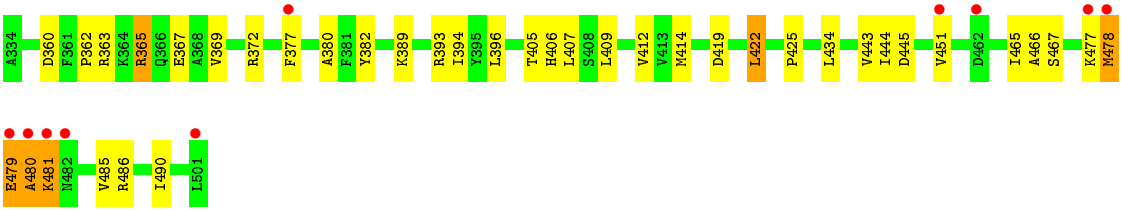
Chain E:





• Molecule 1: TUMOR NECROSIS FACTOR RECEPTOR ASSOCIATED FACTOR 2

Chain F:



• Molecule 2: CD30 PEPTIDE

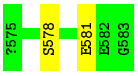
Chain G:

• Molecule 2: CD30 PEPTIDE

Chain H:

• Molecule 2: CD30 PEPTIDE

Chain I:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	91.30Å 110.40Å 91.30Å 90.00° 120.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 37.22 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.00) 89.7 (37.22-2.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.35 (at 2.00Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.220 , 0.244 0.228 , 0.251	Depositor DCC
R_{free} test set	5709 reflections (6.00%)	wwPDB-VP
Wilson B-factor (Å^2)	18.7	Xtriage
Anisotropy	0.196	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 47.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.468 for -h-l,k,h 0.468 for l,k,-h-l 0.081 for h,-k,-h-l 0.079 for -h-l,-k,l 0.079 for l,-k,h	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	8705	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.25% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ACE

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.39	0/1312	0.71	1/1781 (0.1%)
1	B	0.39	0/1312	0.70	1/1781 (0.1%)
1	C	0.38	0/1312	0.70	1/1781 (0.1%)
1	D	0.38	0/1312	0.71	1/1781 (0.1%)
1	E	0.39	0/1312	0.70	1/1781 (0.1%)
1	F	0.37	0/1312	0.71	1/1781 (0.1%)
2	G	0.64	0/59	0.72	0/78
2	H	0.73	0/59	0.81	0/78
2	I	0.67	0/59	0.77	0/78
All	All	0.39	0/8049	0.71	6/10920 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	362	PRO	N-CA-CB	5.72	110.17	103.30
1	B	362	PRO	N-CA-CB	5.71	110.16	103.30
1	D	362	PRO	N-CA-CB	5.64	110.07	103.30
1	A	362	PRO	N-CA-CB	5.59	110.01	103.30
1	E	362	PRO	N-CA-CB	5.58	110.00	103.30
1	F	362	PRO	N-CA-CB	5.49	109.89	103.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1282	0	1238	28	0
1	B	1282	0	1238	27	0
1	C	1282	0	1238	32	0
1	D	1282	0	1238	32	0
1	E	1282	0	1238	29	0
1	F	1282	0	1238	33	0
2	G	62	0	58	2	0
2	H	62	0	58	2	0
2	I	62	0	58	3	0
3	A	145	0	0	5	0
3	B	143	0	0	4	0
3	C	136	0	0	6	0
3	D	116	0	0	2	0
3	E	128	0	0	4	0
3	F	125	0	0	4	0
3	G	14	0	0	0	0
3	H	9	0	0	0	0
3	I	11	0	0	0	0
All	All	8705	0	7602	178	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (178) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:389:LYS:HG2	1:E:414:MET:HE3	1.44	0.98
1:F:389:LYS:HG2	1:F:414:MET:HE3	1.47	0.95
1:F:425:PRO:HG3	1:F:451:VAL:HG13	1.51	0.91
1:E:389:LYS:HG2	1:E:414:MET:CE	2.04	0.88
1:D:389:LYS:HG2	1:D:414:MET:HE3	1.59	0.84
1:C:425:PRO:HG3	1:C:451:VAL:HG13	1.59	0.84
1:A:425:PRO:HG3	1:A:451:VAL:HG13	1.58	0.84
1:F:389:LYS:HG2	1:F:414:MET:CE	2.08	0.83
1:D:389:LYS:HG2	1:D:414:MET:CE	2.09	0.82
1:E:394:ILE:HD11	1:E:407:LEU:HD11	1.63	0.79
1:D:394:ILE:HD11	1:D:407:LEU:HD11	1.64	0.79
1:A:394:ILE:HD11	1:A:407:LEU:HD11	1.66	0.78
1:C:389:LYS:HG2	1:C:414:MET:HE3	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:394:ILE:HD11	1:B:407:LEU:HD11	1.69	0.74
1:A:389:LYS:HG2	1:A:414:MET:HE3	1.69	0.74
1:B:389:LYS:HG2	1:B:414:MET:CE	2.18	0.73
1:A:389:LYS:HG2	1:A:414:MET:CE	2.19	0.73
1:C:389:LYS:HG2	1:C:414:MET:CE	2.20	0.72
1:F:465:ILE:HG13	3:F:9235:HOH:O	1.90	0.71
1:B:389:LYS:HE2	1:B:414:MET:HE3	1.74	0.70
1:F:393:ARG:NH1	2:I:581:GLU:OE1	2.25	0.70
1:B:389:LYS:HG2	1:B:414:MET:HE3	1.72	0.70
1:C:394:ILE:HD11	1:C:407:LEU:HD11	1.74	0.70
1:A:363:ARG:O	1:A:367:GLU:HG3	1.92	0.70
1:F:394:ILE:HD11	1:F:407:LEU:HD11	1.74	0.70
1:B:363:ARG:O	1:B:367:GLU:HG3	1.92	0.69
1:D:393:ARG:NH1	2:G:581:GLU:OE1	2.24	0.69
1:A:389:LYS:HE2	1:A:414:MET:HE3	1.73	0.69
1:D:425:PRO:HG3	1:D:451:VAL:HG13	1.75	0.68
1:C:389:LYS:HE2	1:C:414:MET:HE3	1.75	0.67
1:E:465:ILE:HG13	3:E:9329:HOH:O	1.94	0.67
1:B:478:MET:SD	1:B:479:GLU:N	2.67	0.67
1:C:370:ALA:HB1	1:D:377:PHE:CZ	2.30	0.66
1:C:467:SER:HB3	3:C:9242:HOH:O	1.95	0.66
1:D:451:VAL:HG21	3:D:9815:HOH:O	1.96	0.66
1:F:444:ILE:HG23	3:F:9680:HOH:O	1.95	0.65
1:C:363:ARG:O	1:C:367:GLU:HG3	1.97	0.64
1:D:389:LYS:HE2	1:D:414:MET:HE3	1.80	0.64
1:E:339:GLU:O	1:E:343:LEU:HD13	1.96	0.64
1:F:389:LYS:HE2	1:F:414:MET:HE3	1.81	0.63
1:C:478:MET:SD	1:C:479:GLU:N	2.72	0.62
1:F:467:SER:OG	2:I:578:SER:HB2	1.99	0.62
1:B:482:ASN:HB3	3:B:9190:HOH:O	1.99	0.62
1:A:434:LEU:HB3	1:A:443:VAL:HB	1.81	0.61
1:A:480:ALA:O	1:A:481:LYS:CB	2.49	0.61
1:B:478:MET:O	1:B:480:ALA:N	2.34	0.61
1:E:478:MET:SD	1:E:479:GLU:N	2.74	0.60
1:E:467:SER:OG	2:H:578:SER:HB2	2.01	0.60
1:C:434:LEU:HB3	1:C:443:VAL:HB	1.82	0.60
1:D:482:ASN:HB3	3:D:9647:HOH:O	2.01	0.60
3:C:9057:HOH:O	1:D:377:PHE:HE1	1.85	0.60
1:C:439:ASN:C	1:C:439:ASN:HD22	2.02	0.59
1:E:389:LYS:HE2	1:E:414:MET:HE3	1.84	0.59
1:B:434:LEU:HB3	1:B:443:VAL:HB	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:482:ASN:HB3	3:A:9404:HOH:O	2.02	0.59
1:C:478:MET:O	1:C:480:ALA:N	2.36	0.59
1:A:478:MET:SD	1:A:479:GLU:N	2.76	0.58
1:E:389:LYS:CG	1:E:414:MET:HE3	2.28	0.58
1:F:363:ARG:O	1:F:367:GLU:HG3	2.03	0.58
1:D:363:ARG:O	1:D:367:GLU:HG3	2.04	0.57
1:D:434:LEU:HB3	1:D:443:VAL:HB	1.87	0.56
1:F:377:PHE:HE1	3:F:9101:HOH:O	1.88	0.56
1:D:478:MET:SD	1:D:479:GLU:N	2.79	0.56
1:F:478:MET:SD	1:F:479:GLU:N	2.78	0.56
1:A:479:GLU:C	1:A:481:LYS:H	2.09	0.56
1:A:479:GLU:O	1:A:481:LYS:N	2.39	0.55
1:A:478:MET:O	1:A:480:ALA:N	2.38	0.55
1:D:389:LYS:HG2	1:D:414:MET:HE2	1.88	0.55
1:D:412:VAL:HG22	1:D:466:ALA:HB2	1.88	0.55
1:B:480:ALA:O	1:B:481:LYS:CB	2.55	0.54
1:E:363:ARG:O	1:E:367:GLU:HG3	2.07	0.54
1:F:486:ARG:HH11	1:F:486:ARG:HG3	1.73	0.54
1:D:480:ALA:O	1:D:481:LYS:CB	2.57	0.53
1:E:377:PHE:HE1	3:E:9043:HOH:O	1.89	0.53
1:F:434:LEU:HB3	1:F:443:VAL:HB	1.90	0.53
1:C:372:ARG:NH2	3:C:9537:HOH:O	2.41	0.53
1:F:412:VAL:HG22	1:F:466:ALA:HB2	1.90	0.53
1:A:451:VAL:O	1:A:451:VAL:HG12	2.07	0.53
1:B:479:GLU:C	1:B:481:LYS:H	2.12	0.53
1:C:479:GLU:O	1:C:481:LYS:N	2.35	0.52
1:E:377:PHE:HB2	3:E:9502:HOH:O	2.09	0.52
1:E:480:ALA:O	1:E:481:LYS:CB	2.57	0.52
1:B:412:VAL:HG22	1:B:466:ALA:HB2	1.92	0.52
1:E:419:ASP:HA	1:E:422:LEU:CD2	2.40	0.51
1:C:480:ALA:O	1:C:481:LYS:CB	2.57	0.51
1:F:480:ALA:O	1:F:481:LYS:CB	2.58	0.51
1:B:389:LYS:HG2	1:B:414:MET:HE2	1.90	0.51
1:F:405:THR:OG1	1:F:406:HIS:HD2	1.92	0.51
1:C:451:VAL:O	1:C:451:VAL:HG12	2.09	0.51
1:E:479:GLU:O	1:E:481:LYS:N	2.44	0.51
1:C:339:GLU:O	1:C:343:LEU:HD23	2.10	0.51
1:F:372:ARG:NE	3:F:9505:HOH:O	2.44	0.50
1:E:414:MET:HG2	1:E:463:MET:HG2	1.94	0.50
1:C:482:ASN:HB3	3:C:9512:HOH:O	2.10	0.50
1:D:390:MET:O	1:D:414:MET:HE1	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:476:SER:O	1:A:480:ALA:HB3	2.12	0.50
1:E:376:ILE:HD11	3:E:9497:HOH:O	2.11	0.49
1:E:390:MET:O	1:E:414:MET:HE1	2.12	0.49
1:E:412:VAL:HG22	1:E:466:ALA:HB2	1.95	0.49
1:E:478:MET:O	1:E:480:ALA:N	2.45	0.49
1:B:479:GLU:O	1:B:481:LYS:N	2.38	0.49
1:E:434:LEU:HB3	1:E:443:VAL:HB	1.94	0.49
1:F:466:ALA:HB3	2:I:581:GLU:OE2	2.13	0.49
1:A:389:LYS:HG2	1:A:414:MET:HE2	1.94	0.48
1:A:342:VAL:HG21	1:C:338:LEU:HD11	1.96	0.48
1:C:439:ASN:C	1:C:439:ASN:ND2	2.67	0.48
1:F:479:GLU:O	1:F:481:LYS:N	2.47	0.48
1:D:341:LYS:O	1:D:345:MET:HG3	2.14	0.47
1:D:425:PRO:HG3	1:D:451:VAL:CG1	2.42	0.47
1:E:394:ILE:CD1	1:E:407:LEU:HD11	2.40	0.47
1:F:380:ALA:CB	1:F:414:MET:HE1	2.44	0.47
1:C:479:GLU:C	1:C:481:LYS:H	2.18	0.47
1:D:486:ARG:HG3	1:D:486:ARG:HH11	1.79	0.47
1:C:451:VAL:O	1:C:451:VAL:CG1	2.62	0.47
1:F:377:PHE:CZ	1:F:393:ARG:NE	2.77	0.47
1:A:372:ARG:NH2	3:A:9425:HOH:O	2.46	0.47
1:D:478:MET:O	1:D:480:ALA:N	2.47	0.47
1:E:419:ASP:HA	1:E:422:LEU:HD22	1.97	0.47
1:C:439:ASN:O	1:C:439:ASN:ND2	2.48	0.47
1:D:419:ASP:HA	1:D:422:LEU:CD2	2.45	0.46
1:A:372:ARG:CG	3:A:9271:HOH:O	2.63	0.46
1:F:396:LEU:HA	1:F:407:LEU:HD12	1.97	0.46
1:A:366:GLN:HB3	3:A:9425:HOH:O	2.16	0.46
1:A:372:ARG:HD3	3:A:9271:HOH:O	2.14	0.46
1:F:389:LYS:CG	1:F:414:MET:HE3	2.30	0.46
1:B:372:ARG:CG	3:B:9266:HOH:O	2.63	0.46
1:A:486:ARG:HD2	3:C:9470:HOH:O	2.15	0.46
1:D:339:GLU:O	1:D:343:LEU:HD13	2.16	0.46
1:C:370:ALA:HB3	1:C:372:ARG:HD3	1.99	0.45
1:E:389:LYS:HG2	1:E:414:MET:HE2	1.96	0.45
1:C:361:PHE:O	1:C:365:ARG:HB2	2.17	0.45
1:C:382:TYR:CD1	1:C:382:TYR:N	2.85	0.45
1:B:482:ASN:N	3:B:9643:HOH:O	2.49	0.45
1:A:454:SER:HA	1:A:457:GLN:HG2	1.99	0.44
1:B:361:PHE:O	1:B:365:ARG:HB2	2.18	0.44
1:D:414:MET:HG2	1:D:463:MET:HG2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:486:ARG:HG3	1:C:486:ARG:HH11	1.82	0.44
1:F:396:LEU:HA	1:F:407:LEU:CD1	2.47	0.44
1:F:485:VAL:HG22	1:F:490:ILE:CG2	2.48	0.44
1:A:451:VAL:O	1:A:451:VAL:CG1	2.65	0.44
1:B:382:TYR:CD1	1:B:382:TYR:N	2.85	0.44
1:F:451:VAL:HG12	1:F:451:VAL:O	2.17	0.44
1:B:394:ILE:CD1	1:B:407:LEU:HD11	2.42	0.43
1:B:437:GLN:CD	1:B:486:ARG:HB3	2.39	0.43
1:A:486:ARG:HG3	1:A:486:ARG:HH11	1.83	0.43
1:B:414:MET:HG2	1:B:463:MET:HG2	2.00	0.43
1:F:419:ASP:HA	1:F:422:LEU:HD22	2.01	0.43
1:A:438:ASN:HB2	1:A:483:SER:HB2	2.00	0.43
1:B:476:SER:O	1:B:480:ALA:HB3	2.19	0.43
1:F:365:ARG:O	1:F:369:VAL:HG23	2.18	0.43
1:F:478:MET:O	1:F:480:ALA:N	2.52	0.42
1:D:466:ALA:HB3	2:G:581:GLU:OE2	2.18	0.42
1:D:382:TYR:N	1:D:382:TYR:CD1	2.87	0.42
1:E:382:TYR:CD1	1:E:382:TYR:N	2.88	0.42
1:B:338:LEU:HD11	1:C:342:VAL:HG21	2.01	0.42
1:C:370:ALA:CB	1:C:372:ARG:HD3	2.49	0.42
1:B:458:ARG:HA	1:B:459:PRO:HD3	1.92	0.42
1:B:473:CYS:HA	1:B:474:PRO:HD3	1.95	0.42
1:B:474:PRO:HD3	3:B:9458:HOH:O	2.20	0.42
1:B:469:CYS:HA	1:B:470:PRO:HD2	1.96	0.41
1:C:414:MET:HG2	1:C:463:MET:HG2	2.01	0.41
1:D:405:THR:OG1	1:D:406:HIS:HD2	2.03	0.41
1:D:394:ILE:CD1	1:D:407:LEU:HD11	2.41	0.41
1:A:389:LYS:CG	1:A:414:MET:HE3	2.46	0.41
1:D:419:ASP:HA	1:D:422:LEU:HD22	2.02	0.41
1:E:365:ARG:NH2	1:E:475:VAL:HG11	2.36	0.41
1:D:478:MET:SD	1:D:479:GLU:CB	3.08	0.41
1:E:466:ALA:HB3	2:H:581:GLU:OE2	2.20	0.41
1:F:382:TYR:N	1:F:382:TYR:CD1	2.88	0.41
1:A:382:TYR:N	1:A:382:TYR:CD1	2.88	0.41
1:E:437:GLN:NE2	1:E:486:ARG:HB3	2.35	0.41
1:C:414:MET:SD	3:C:9350:HOH:O	2.63	0.41
1:D:485:VAL:HG22	1:D:490:ILE:CG2	2.50	0.41
1:C:436:ASP:OD1	1:C:483:SER:HB2	2.22	0.40
1:D:389:LYS:CG	1:D:414:MET:HE3	2.41	0.40
1:E:396:LEU:HA	1:E:407:LEU:CD1	2.51	0.40
1:F:377:PHE:CE1	1:F:393:ARG:NE	2.80	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:444:ILE:HG12	1:F:445:ASP:N	2.35	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	166/168 (99%)	154 (93%)	7 (4%)	5 (3%)	4 1
1	B	166/168 (99%)	155 (93%)	6 (4%)	5 (3%)	4 1
1	C	166/168 (99%)	155 (93%)	6 (4%)	5 (3%)	4 1
1	D	166/168 (99%)	156 (94%)	6 (4%)	4 (2%)	6 2
1	E	166/168 (99%)	158 (95%)	3 (2%)	5 (3%)	4 1
1	F	166/168 (99%)	157 (95%)	4 (2%)	5 (3%)	4 1
2	G	7/9 (78%)	7 (100%)	0	0	100 100
2	H	7/9 (78%)	7 (100%)	0	0	100 100
2	I	7/9 (78%)	7 (100%)	0	0	100 100
All	All	1017/1035 (98%)	956 (94%)	32 (3%)	29 (3%)	4 1

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	479	GLU
1	A	480	ALA
1	A	481	LYS
1	B	479	GLU
1	B	480	ALA
1	B	481	LYS
1	C	477	LYS

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Mol	Chain	Res	Type
1	C	479	GLU
1	C	480	ALA
1	C	481	LYS
1	D	477	LYS
1	D	481	LYS
1	E	477	LYS
1	E	481	LYS
1	F	477	LYS
1	F	481	LYS
1	A	477	LYS
1	B	477	LYS
1	E	479	GLU
1	E	480	ALA
1	F	479	GLU
1	F	480	ALA
1	B	478	MET
1	C	478	MET
1	D	479	GLU
1	D	480	ALA
1	E	478	MET
1	A	478	MET
1	F	478	MET

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	132/145 (91%)	129 (98%)	3 (2%)	50	53
1	B	132/145 (91%)	128 (97%)	4 (3%)	41	41
1	C	132/145 (91%)	128 (97%)	4 (3%)	41	41
1	D	132/145 (91%)	127 (96%)	5 (4%)	33	31
1	E	132/145 (91%)	129 (98%)	3 (2%)	50	53
1	F	132/145 (91%)	128 (97%)	4 (3%)	41	41
2	G	7/7 (100%)	7 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	H	7/7 (100%)	7 (100%)	0	100 100
2	I	7/7 (100%)	7 (100%)	0	100 100
All	All	813/891 (91%)	790 (97%)	23 (3%)	43 44

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	365	ARG
1	A	409	LEU
1	A	422	LEU
1	B	365	ARG
1	B	366	GLN
1	B	409	LEU
1	B	422	LEU
1	C	365	ARG
1	C	409	LEU
1	C	422	LEU
1	C	439	ASN
1	D	360	ASP
1	D	365	ARG
1	D	366	GLN
1	D	409	LEU
1	D	422	LEU
1	E	365	ARG
1	E	409	LEU
1	E	422	LEU
1	F	360	ASP
1	F	365	ARG
1	F	409	LEU
1	F	422	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	366	GLN
1	A	406	HIS
1	A	427	ASN
1	A	461	ASN
1	B	366	GLN
1	B	406	HIS

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Mol	Chain	Res	Type
1	B	461	ASN
1	C	406	HIS
1	C	439	ASN
1	C	461	ASN
1	D	406	HIS
1	D	461	ASN
1	E	366	GLN
1	E	406	HIS
1	E	439	ASN
1	F	406	HIS
1	F	461	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	168/168 (100%)	-0.04	5 (2%) 50 49	12, 20, 44, 51	0
1	B	168/168 (100%)	-0.08	5 (2%) 50 49	11, 20, 42, 51	0
1	C	168/168 (100%)	-0.11	4 (2%) 59 57	12, 20, 42, 52	0
1	D	168/168 (100%)	-0.03	6 (3%) 42 42	12, 21, 37, 51	0
1	E	168/168 (100%)	-0.08	7 (4%) 36 35	12, 21, 38, 51	0
1	F	168/168 (100%)	-0.04	10 (5%) 21 20	12, 21, 37, 52	0
2	G	8/9 (88%)	-0.19	0 100 100	16, 18, 25, 30	0
2	H	8/9 (88%)	-0.36	0 100 100	15, 18, 25, 29	0
2	I	8/9 (88%)	-0.23	0 100 100	16, 18, 26, 30	0
All	All	1032/1035 (99%)	-0.07	37 (3%) 42 42	11, 20, 42, 52	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	480	ALA	7.0
1	D	478	MET	5.8
1	B	480	ALA	5.2
1	A	480	ALA	5.2
1	E	478	MET	4.9
1	D	480	ALA	4.7
1	F	480	ALA	4.6
1	F	481	LYS	4.3
1	D	481	LYS	4.0
1	A	478	MET	3.8
1	F	478	MET	3.6
1	C	478	MET	3.4
1	A	479	GLU	3.2
1	C	480	ALA	3.0
1	A	481	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	482	ASN	3.0
1	E	377	PHE	2.9
1	D	438	ASN	2.9
1	B	334	ALA	2.9
1	C	482	ASN	2.7
1	F	482	ASN	2.7
1	B	478	MET	2.7
1	D	451	VAL	2.7
1	F	451	VAL	2.6
1	E	477	LYS	2.5
1	C	439	ASN	2.5
1	F	477	LYS	2.4
1	B	482	ASN	2.4
1	F	462	ASP	2.4
1	E	438	ASN	2.3
1	F	501	LEU	2.3
1	D	482	ASN	2.2
1	B	479	GLU	2.2
1	F	479	GLU	2.2
1	E	334	ALA	2.2
1	E	462	ASP	2.1
1	F	377	PHE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.